

Quantum recognition of eigenvalues, structure of devices and thermodynamic properties

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Abstract

Quantum algorithms speeding up classical counterparts are proposed for the problems:

1. Recognition of eigenvalues with fixed precision. Given a quantum circuit generating unitary mapping U and a complex number the problem is to determine is it an eigenvalue of U or not.
2. Given a molecular structure find thermodynamic functions like partitioning function, entropy, etc. for a gas consisting of such molecules.
3. Recognition of molecular structures. Find a molecular structure given its spectrum.
4. Recognition of electronic devices. Given an electronic device that can be used only as a black box how to recognize its internal construction?

We consider mainly structures generating sparse spectrums. These algorithms require the time from about square root to logarithm of the time of classical analogs and for the first three problems give exponential memory saving. Say, the time required for distinguishing two devices with the same given spectrum is about seventh root of the time of direct classical method, for the recognition of eigenvalue - about sixth root. Thus microscopic quantum devices can recognize molecular structures and physical properties of environment faster than big classical computers.

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1 Electronic devices and quantum computations

1.1 Statements of problems and outline of the work

The aim of this paper is to build effective quantum algorithms for the problems of the following types:

- Given a quantum gate array generating unitary operator U and a complex number ω how to determine is it an eigenvalue of U or not (precision of determining eigenvalues is fixed)?
- How to recognize a structure of unknown electronic or molecular device given only access to its function?

Here the first problem will be an important intermediate step in the solution of the second¹. Consider them sequentially.

Recognition of eigenvalues. This problem is closely connected with finding of eigenvalues distribution or density of states (DOS) that is energy levels $E_0 < E_1 < \dots$ and dimensions of the corresponding subspaces d_0, d_1, \dots . DOS plays a key role in calculation of thermodynamic functions given by

$$F = \sum_j a(j) d_j e^{-\frac{E_j}{k_B T}} \quad (1)$$

for some values $a(j)$ so that the summands quickly converge to zero. Say, if all $a(j) = 1$ this expression gives the partition function Q , if $a(j) = E_j/Q$ it gives an average energy, if

¹A straightforward calculation shows that the simulation of evolution generated by a given Hamiltonian up to a time instant τ with a fixed accuracy requires of order τ^2 steps on a quantum computer. This means that all results of the paper can be generalized to arbitrary quantum systems. This subject will be elaborated in more details in another paper.

$a(j) = -\frac{k_B}{Q} \ln(e^{-E_j/k_B T}/Q)$ - an entropy. Having an efficient method of finding d_j we would be able to obtain thermodynamic functions and to determine important properties of environment consisting of such molecules like heat capacity. The best known classical method of finding DOS was proposed by Hams and Raedt in the work [HR]. Their method requires the time of order dimension N of the space of states and the memory of the same order (whereas the direct method of calculation eigenvalues requires the time of order N^3). The first quantum algorithm for this problem proposed by Abrams and Lloyd in [AL] requires the same time $O(N)$ and logarithmic memory. The method proposed in the present work requires the time of order square root of classical and memory of order $\ln^2 N$.

The idea of our approach is the following. We shall use combination of Grover search algorithm (GSA), revealing eigenvalues by Abrams and Lloyd method ([AL]) and universal quantum function of application App. Abrams and Lloyd method of revealing eigenvalues is based on the application of U controlled by ancillary qubit α as

$$U_{cond}|x, \alpha\rangle \longrightarrow \begin{cases} |Ux, \alpha\rangle, & \text{if } \alpha = 1, \\ |x, \alpha\rangle & \text{if } \alpha = 0. \end{cases}$$

Note that it is the direct generalization of Shor's trick which can be obtained if U is a multiplication by a given integer modulo q ([Sh]).

Recognition of devices structure.

We shall tell apart two versions of this general problem: the recognition of molecular structures and the recognition of electronic circuits.

If we want to determine a molecular structure then it is natural to assume that its functionality is given as the spectrum of its Hamiltonian, e.g. the set of its energy levels. Thus here it is required to find a quantum system whose Hamiltonian has a given spectrum.

The problem of recognition of electronic circuits is stated otherwise. An electronic device is thought of as a source of electromagnetic fields which can control some quantum system Q . Let such a field induces evolution of the system with Hamiltonian H in time frame δt . Thus we have a correspondence: electronic device \longrightarrow Hamiltonian, δt . Evolution of a quantum system Q induced by this Hamiltonian can be presented as a unitary transform $U = e^{-\frac{i}{\hbar} H \delta t}$. Then, given a device C and a value of time t we can associate with it some unitary transformation U_C . Assume that we have recognized a circuit C if we find some circuit C_1 such that $U_C = U_{C_1}$ with high accuracy. We shall write U instead of U_C for the circuit C that we want to recognize. But in fact we shall solve the more general problem when a tested device C can be used as a black box acting on n qubits as a function U_C so that if x is an input then $U_C|x\rangle$ is a result of its action on this input. Here a tested device can contain its own quantum memory and it can be entangled with Q in course of fulfilling U but this entanglement must be then eliminated. The existence of such entanglement means that this case cannot be described by the Hamiltonian of system Q . For the simplicity we assume that an unknown circuit is built of elementary functional elements from some fixed set $\{E_1, E_2, \dots, E_o\}$. The next natural assumption is that a size of circuit is limited by some constant c so that our circuit is some unknown combination of c functional elements. Denote by \mathcal{E} all circuits of the length c . We can encode such $C \in \mathcal{E}$ by a string $[C]$ of ones and zeroes so that decoding procedure is easy as well and we can immediately

recreate a circuit given its code. Thus we can look through all circuits looking through its codes. The same coding can be built for electronic devices.

A straightforward solution of the problems is clear. For the problem of recognition of molecular structures all that we need is to be able to recognize eigenvalues of transformation generated by a given circuit. Each eigenvalue of unitary operator has the form $e^{2\pi i\omega}$ where ω is a real number from $[0, 1)$ called frequency. In what follows by spectrum we mean a set of all frequencies. Let all frequencies are grouped near points of the form $\frac{l}{M}$ where M is not very big, $l = 0, 1, \dots, M - 1$. Assume that the acceptable precision of recognition of frequencies is $1/M$. Then having an algorithm for eigenvalue recognition we can apply it again and again constructing spectrums generated by all possible circuits and thus find a wanted circuit with given spectrum. If we need to recognize a circuit of electronic device we can examine all possible circuits taken in some order. Examination of one circuit means that we run it on all possible inputs one after another and compare the results with the corresponding result of a tested device action.

For the problem of recognition of molecular structures our method requires the time of order sixth root of the time of direct classical method whereas memory saving is exponential. For the problem of recognition of electronic circuits our method gives at least square root time saving in the case when classical counterparts exist (this is the narrow formulation when a tested device generates classical mapping). But in general case an advantage may be more. For example we can tell apart two devices with the same spectrum in the time about seventh root of the time of naive brut force.

To recognize devices quantumly we must be able to store and fulfill operations on the codes of different circuits. This possibility is based on the existence of a quantum analog of the universal Kline function. This is a unitary operator App such that for all quantum devices C and all inputs x $\text{App}|x, [C]\rangle = |U_C x, [C]\rangle$. We assume that for the wide range of quantum devices C with c particles C may be encoded as integer $[C]$ in time $O(c)$ so that the quantum complexity of App is $O(c)$ as well.

We shall consider here a particular case of the problem when all eigenvalues of U are known a-priori or can be obtained beforehand. This restriction is not yet very constraining. To illustrate what kind of tasks we shall be able to solve by the proposed method consider a few examples of the problem of recognition of an electronic device whose spectrum is known.

Recognition of quantum algorithms designed as subroutines. Such algorithms must restore an input if we apply it twice. Computing a function f they act as $|x, b\rangle \longrightarrow |x, b + f(x) \bmod 2\rangle$. All known quantum algorithms can be presented in such form. For such quantum algorithms their unitary transformation U has only two eigenvalues: 1 and -1 . Given a controlling device for such algorithm (it may include classical elements and ancillary qubits as well) we can quickly recognize its construction. Alternatively, we can quickly find quantum or classical algorithm for a given task.

Consider a "classical" particular case of the recognition problem when U maps each basic state to a basic state which means that the matrix of U consists of ones and zeroes and in addition U equals U^{-1} . Here evident strategy of recognition takes of order $\text{card}(\mathcal{E})2^n$ steps. This case of the problem may be reformulated as the finding of such t that for all s some given predicate $A(t, s)$ is true. This is the problem of verification of logical formulas. Quantum

solution of it in a time about square root of classical time based plainly on Grover's trick was proposed in [BCW]. This method doesn't work in the general case where U_C is arbitrary involutive unitary transform, e.g. such that $U = U^{-1}$. Just this general case is the subject of this work. Here we cannot recognize a circuit so easy as in "classical" case because it is difficult to compare two quantum states $U_C|x\rangle$ and $U|x\rangle$.

The general idea of our approach to the recognition of arbitrary electronic devices is the following. We shall include a device C which structure we want to recognize into a classical controlling part of quantum computer. Thus a tested device generates unitary transformation on n qubit system. Then reveal eigenvectors of U using U_{cond} by the method mentioned above and compare them with eigenvectors of circuits from \mathcal{E} choosing a circuit giving the best approximation. Here GSA will be used in the last step and in the several intermediate steps.

Assumption about sparse spectrum

In this paper we shall consider mainly circuits generating sparse spectrums. It means that spectrums of operators U_C are so designed that the frequencies are grouped into groups such that a minimal distance between frequencies from the different groups is more than $1/M$ and a maximal distance between frequencies from the same group is less than $1/L$. For the problems of eigenvalues and molecular structures recognition we require that $L = 16M$ that is not yet very restricting. For the recognition of electronic devices we shall suppose $L \gg M$ that is more strong limitation. Spectrums are called sparse if $M = const$ when $N \rightarrow \infty$. For sparse spectrums our algorithms show the best performance.

Spectrums that are not sparse are called dense. For dense spectrums our methods give the less advantage over classical algorithms (look at section 3.6). An example of dense spectrum: $\omega_k = \frac{k}{N}$, $k = 0, 1, \dots, N-1$. The similar problems for dense spectrums will be studied in one of the following papers.

We write $\omega' \approx \omega$ iff ω' and ω belong to the same group. For the simplicity assume also that for each group of frequencies there exists a number of the form l/M disposed between some two frequencies of this group where l is an integer less than M .

1.2 An abstract model of QC. "Plug and play" technology

To build algorithms recognizing circuits we need an abstract model of quantum computer (QC). QC consists of two parts: quantum and classical. Classical part exactly determines what unitary transformation must be fulfilled at each time instant with quantum part and thus plays a role of controller for it. These unitary transformations are of two sorts: working transformations - which our computer performs itself and query transformations - induced by a tested device: U or U_{cond} .

We can suppose that a quantum part Q consists of nuclear spins or interacting dipoles (or some other quantum two levels systems) and a classical part is a source of electromagnetic fields determining evolution of a quantum part. The general form of a state of quantum part will be $\chi = \sum_{i=0}^{2^\nu-1} \lambda_i e_i$ where the basic states of it $e_0, \dots, e_{2^\nu-1}$ are simply strings of ones and zeroes of the length ν where $\nu > n$ is the size of quantum part which can contain some auxiliary qubits behind input for U , $\sum_{i=0}^{2^\nu-1} |\lambda_i|^2 = 1$, $N = 2^n$ is the number of all classical input words for U .

Classical part determines when to "switch on" a tested device (usually it happens many times) and when to observe a result of computation. Observation of a state χ gives every basic state e_i with the corresponding probability $|\lambda_i|^2$.

The problem of recognition of electronic devices presumes the so-called "plug and play" technology where a tested device is applied only as a black box. If query transformations are only U then our model evidently satisfies requirements of "plug and play" technology where we classically control when to switch on a tested device. An implementation of U_{cond} in the framework of this technology is not so easy because it requires a quantum control on applications of the device ². Nevertheless it is possible to implement U_{cond} in the framework of "plug and play" technology. This possibility will be substantiated in the following papers. Now we shall simply presume that it is possible. Such difficulty does not exist for the problems of eigenvalue and molecular structures recognition. Here we can manage without oracles at all because having an explicit form of a quantum gate array realizing a universal function of application App we can quantumly control its actions in each element separately and simultaneously thus implementing U_{cond} .

Let every basic state be partitioned as:

$e_i = |\text{place for code } [C], R_{\bar{1}}, R_{\bar{2}}, \dots, R_{\bar{l}}\rangle$, where each register $R_{\bar{i}}$ in its turn is partitioned into a place for argument, places for time instants and places for the corresponding frequencies. Here a complex index \bar{i} contains one or two integers so that the length of e_i is polynomial of c and n of at most second degree.

2 Obtaining new algorithms from basic quantum tricks

2.1 GSA and amplitude amplification

GSA proposed in ([Gr]) is one of two basic quantum tricks. It is meant for quick getting of a quantum state \bar{a} given the inversion along this state $I_{\bar{a}}$. An inversion along some state \bar{a} is defined by

$$I_{\bar{a}}|\bar{x}\rangle = \begin{cases} |\bar{x}\rangle, & \text{if } x \perp a, \\ -|\bar{a}\rangle, & \text{if } x = a. \end{cases}$$

We also assume that $I_{\bar{a}}$ acts like identity if \bar{a} does not exist. A typical situation is when a state is unknown but the inversion along it can be fulfilled easily. Say, let \bar{a} be a solution of equation $f(x) = 1$ with a simply computable Boolean function f . Then the inversion $I_{\bar{a}}$ can be implemented by addition modulo 2 of $f(x)$ to an ancillary qubit initialized by $\frac{|0\rangle - |1\rangle}{\sqrt{2}}$. This transformation maps a state $|x, \frac{|0\rangle - |1\rangle}{\sqrt{2}}\rangle$ to the same state with the sign $+$ or $-$ subject to the satisfaction of equality $f(x) = 1$. The transformation is unitary and can be easily fulfilled given a device fulfilling f . All sequential transformations in our formulas will be applied from right to left.

GSA is sequential applications of the transformation $G = I_{\bar{a}}I_0$ to a state $\tilde{0}$ which is chosen randomly beforehand. If we apply this transformation $O(\sqrt{N})$ times where N is the dimension

²This would be evidently possible provided we have access to the internal details of our device and can quantumly control their work simultaneously. But this assumption contradicts to "plug and play" technology.

of main space then an observation of quantum part yields \bar{a} with visible probability whereas without quantum computer we would be compelled to spend of order N steps to find \bar{a} .

A little difficulty here is that we don't know exactly a time instant t when to stop iterations to make probability of error negligible that is needed when applying GSA as subroutine. Here the following simple trick helps.

Define a number $B = B(N)$ so that $1/B$ is an average value of $|\langle a | \tilde{0} \rangle|$ for $\tilde{0}$ uniformly distributed on a sphere of radius 1 in the space of inputs. A straightforward calculation shows that $B = O(\sqrt{N})$. Let GenArg_j be operators generating arbitrary vectors \bar{a}_j from the space of inputs belonging to independent uniform distributions, $j \in \{1, 2, \dots, k\}$, and let GenTimeArg_j be operators generating time instants t_j from independent uniform distributions on integers from the segment $[0, B]$. Arrange k copies of two working registers: for input and for storage of a time instant and fulfill the corresponding operator $(I_{\tilde{0}} I_{\bar{a}})^{t_j} \text{GenArg}_j \text{GenTime}_j$ on each register. Now if \bar{a} exists then the probability to obtain \bar{a} observing any one register is at least $1/4$ (it is shown in [BBHT]) and the probability to obtain any fixed other state will be negligible because our operators GenArg_j generate independent uniformly distributed samples. If \bar{a} does not exist which means that $I_{\bar{a}}$ is identity then the probability to obtain any fixed state will be negligible. Denote by \bar{a}_j the contents of j -th register for argument in the resulting state. Consider the following criterion: if at least one fifth of \bar{a}_j , $j = 1, 2, \dots, k$ coincide then we decide that \bar{a} is this value, if not then \bar{a} does not exist. Calculate the error probability of this criterion. Let K be a number of such j that $\bar{a}_j = \bar{a}$. By the central limit theorem the probability that a fraction $\frac{(k/4) - K}{\sqrt{(k/4) \cdot (3/4)}}$ belongs to the segment $[\alpha_1, \alpha_2]$ is closed to $\frac{1}{\sqrt{2\pi}} \int_{\alpha_1}^{\alpha_2} e^{-\frac{x^2}{2}} dx$. Then the straightforward calculations give that the probability of that $K \leq k/5$ will be of order $\int_{\alpha_1}^{\infty} e^{-\frac{x^2}{2}} dx$ for α_1 of order \sqrt{k} . Thus to make error probability of order $1/\sqrt{N}$ it would suffice to choose k of order $n = \log N$. This method can be used not only for GSA but also for other algorithms. If a probability to obtain a right result for each of k registers is some positive p which does not depend on the dimensionality then to make this probability $1/N_1$ it is sufficient to choose k of order $\log N_1$. In what follows we shall use this simple trick without special mentioning and will mark the simultaneous operations of the same kind on all working registers by \bigotimes_j . We assume that all ensembles generated by the different j -th copies of operators are taken from the independent distributions.

We shall use the standard norm on operators in Hilbert space defined by $\|A\| = \sup_{\|\bar{x}\|=1} \|A\bar{x}\|$.

Given an operator A denote by A_ϵ such operator A' that $\|A - A'\| \leq \epsilon$. In what follows we shall use a simple trick described above making necessary copies of registers and so will raise an accuracy of our operators up to required level. When we must repeat an operator T times the required accuracy of one application must be $1/T$ and it may be ensured by only linear price in memory as it was shown above. This means that we shall always use A_ϵ instead of A without special mentioning where $\epsilon = O(1/T)$ if an operator A must be repeated T times.

2.2 Revealing of eigenvalues

The second basic quantum trick is designed to reveal eigenvalues of a given unitary operator U . We shall define an operator revealing frequencies in accordance to the work [AL].

Let $M = 2^m, L = 2^p$. We are going to determine frequencies of unitary operators in within $1/L$ where L is a number of applications of U required for the revelation of frequencies with this accuracy which means that $1/M$ is an accuracy that is sufficient to tell apart eigenvalues of U . For the recognition of eigenvalues we put $p = m + 4$ so that $L = 16M$.

Denote by $(0.l)_p$ a number from $[0, 1)$ of the form l/L . Let an operator U have eigenvalues $e^{2\pi i \omega_k}$ where frequencies $\omega_0, \omega_1, \dots, \omega_{N'-1}$ are the different real numbers from $[0, 1)$. Denote by E_k the space spanned by all eigenvectors corresponding to ω_k . An arbitrary vector with the length 1 from E_k will be denoted by Φ_k . Thus every state ξ has the form $\xi = \sum_{k=0}^{N'-1} x_k \Phi_k$.

Let $\Omega = \{\tilde{\omega}_{k,i}\}$ be some set of integers from $\{0, 1, \dots, L-1\}$, $0 \leq i \leq \mathcal{M}-1$, $0 \leq k \leq N'-1$; $\varepsilon, \delta > 0$. Denote $L_\varepsilon^k(\Omega) = \{i : |(0.\tilde{\omega}_{k,i})_p - \omega_k| \leq \varepsilon \text{ or } |(0.\tilde{\omega}_{k,i})_p - \omega_k - 1| \leq \varepsilon\}$.

Definition 1 A transformation W of the form

$$W : |\xi, 0^{m+4}\rangle \longrightarrow \sum_{k=0}^{N'-1} \sum_{i=0}^{L-1} \lambda_{i,k} |\Phi_k, \tilde{\omega}_{k,i}\rangle$$

is called a transformation of $W_{\delta,\varepsilon}$ type if for all k and ξ $\sum_{i \in L_\varepsilon^k(\Omega)} |\lambda_{i,k}|^2 \geq |x_k|^2 (1 - 2\delta)$.

Thus, δ is an error probability of getting right frequencies ω_k by observation of the second register, and ε is a precision of frequencies approximations.

Definition 2 A unitary operator R is called revealing frequencies of U if R belongs to the type $W_{\frac{1}{K}, \frac{K}{L}}$ for any $K \in \{1, 2, \dots, L\}$.³

The key here is the quantum version of Fourier transform defined by

$$\text{QFT}_L : |s\rangle \longrightarrow \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} e^{\frac{-2\pi i s l}{L}} |l\rangle$$

We need also the following generalization U_{seq} of operator U_{cond} :

$$U_{seq}^L |x, a\rangle = |U^a x, a\rangle.$$

This is the result of a sequential applications of U to the main register. To implement this operator by means of U_{cond} fulfill the following cycle. For integer counter j altering from 1 to the maximal value $L-1$ of a apply U iff $j \leq a$. Then one cycle consists of U_{cond} with a properly prepared controller and the resulting operator will be U_{seq}^L .

Define an operator revealing frequencies by

$$\text{Rev} = \text{QFT}_L U_{seq}^L \text{QFT}_L,$$

³in what follows we shall use this notion only with $K = 16$.

where quantum Fourier transforms are applied to the second register ⁴. In the work [Oz] it was proved that Rev is a transformation revealing frequencies. Now we need more. For the redistribution of amplitudes x_k we shall need also a transformation Rest cleaning the second register. An ideal candidate for this role would be Rev^{-1} but a problem is that it requires an application of U^{-1} that is physically unrealizable given only device fulfilling U excluding evident cases where say $U = U^{-1}$. We can use this easiest definition of Rest only in case when we are given a circuit implementing U (say, gate array) because then U^{-1} is accessible for us as well as U . But if C is given only as a black box then the restoring operator should be defined separately.

We shall find an operator restoring ancilla in the form

$$\text{Rest} = \text{Rev}D$$

where D is some operator of turning.

Let we are given some integers $\tilde{\omega}_k^L$ of the form $\frac{q}{L}$, q - integer, $\tilde{\omega}_k^L \approx \omega_k$. Then we could define an operator of turning D by $D|\Phi_k, l\rangle = e^{-2\pi i(L-1)\delta_{k,l}}|\Phi_k, l\rangle$ where $\delta_{k,l} = \tilde{\omega}_k^L - (0.l)_m$. It was proved in [Oz] that $\|(\text{RestRev}|\chi, \bar{0}\rangle - |\chi, \bar{0}\rangle)\| < 7M/L$ which means that so defined restoring operator really restores zeroes in the second register after action of Rev provided L is large enough. To create these good approximations we apply a bit more general construction. Put

$$D = \text{Enh } \tilde{D} \text{ Enh}$$

where an operator Enh calculates an integer function $h(l)$ giving a good approximation $(0.h(l))_p$ of frequencies in within $1/L$ given their rough approximation $(0.l)_m$ in within $1/M$ and places them into ancilla, \tilde{D} turns each eigenvector on appropriate angle:

$\tilde{D}|\Phi_k\rangle = e^{-2\pi i(M-1)((0.h(l))_p - (0.l)_p)}|\Phi_k$ and the last application of Enh cleans ancilla. An operator Enh is accessible given good approximations of eigenvalues. Thus our operator Rest restores zeroes in ancilla in within $1/L$.

We can reach an accuracy $1/L$ of all operators of type Rest that will be less than $1/t$ where t is the number of all steps in computation and this accuracy can be guaranteed with $\log L = p$ registers. Emphasize that this difficulty with eigenvalue precision arises only when U^{-1} is inaccessible - in the problem of recognition of electronic circuits in the section 3.4 where we must choose $L \gg M$.

Operators Rev and Rest can be built in the form of quantum gate array using universal quantum Klini function App where a code $[C]$ of circuit generating U is a part of input. We shall write the operator U corresponding to these two operators as its upper index.

3 Problems of recognition

3.1 Getting eigenvectors and recognition of eigenvalues

Our assumption about sparse spectrum now is stated as $L = 16M = \text{const}$. In view of that Rev reveals frequencies it belongs to the type $W_{\frac{1}{16}, \frac{1}{M}}$. By the definition of $W_{\delta, \varepsilon}$ it means that

⁴the first QFT can be replaced by Walsh-Hadamard transform as in [AL] because on zero ancilla it is equivalent

Rev gives a state $\sum_{k=0}^{N'-1} \sum_{i=0}^{M-1} \lambda_{i,k} |\Phi_k, \tilde{\omega}_{k,i}\rangle$ where the seven eighth of probability is concentrated on such pairs i, k that $(0.\omega_{i,k})_m$ is closed to ω_k . This means that we can get eigenvalues with high probability observing the second register whereas the first register will contain the corresponding eigenvector. This way of getting eigenvectors was proposed in the papers [AL, TM]. The first disadvantage of it is irreversibility. Observing a state we lose full information about it and cannot use this state again that is very important for building of nontrivial quantum algorithms. The second disadvantage is that this way gives a random eigenvector when it is typically required to obtain the eigenvector corresponding to a given frequency.

Let we are given a good approximation $\tilde{\omega}^L$ of some frequency ω written as a string of p its sequential binary figures and let $\mathcal{E}_\omega = \{\Phi_1^\omega, \dots, \Phi_l^\omega\}$ be a basis of the subspace E_ω of eigenvectors corresponding to all frequencies $\omega' \approx \omega$. We shall build an operator State_ω which concentrates the bulk of amplitude on some superposition of the corresponding eigenvectors: $\sum_{j=1}^l \lambda_j \Phi_j^\omega \in E_\omega$. For this aim we are going to apply GSA. Let $|\bar{a}\rangle$ be some randomly chosen vector from the main space: $|\bar{a}\rangle = \sum_{j=1}^l \mu_j \Phi_j^\omega + \sum_s \nu_s \Phi_s$ where all eigenvectors from the second sum correspond to frequencies $\omega' \not\approx \omega$. Here our target state will be the following vector $E_\omega(\bar{a}) = \sum_{j=1}^l \lambda_j \Phi_j^\omega$ where $\lambda_j = \frac{\mu_j}{\sqrt{\sum_{j=1}^l |\mu_j|^2}}$, that is a vector of the length 1 directed along the projection of \bar{a} to subspace E_ω .

Let A be some set of vectors. We denote by I_A an operator changing the sign of all vectors from A and remaining unchanged all vectors orthogonal to A . We need to obtain the operator I_{E_ω} constrained to the two dimensional subspace $S(\bar{a}, \omega)$ spanned by vectors $|\bar{a}\rangle$ and $E_\omega(\bar{a})$.

Let Rev_j , Rest_j be j -th copies of the operators Rev, Rest acting on the corresponding places of j -th register. Denote by l_j a string contained in the place for frequency of j -th register. Put

$$\tilde{I}_{E_\omega} = \bigotimes_j^v \text{Rest}_j \text{Sign}_\omega \bigotimes_j^v \text{Rev}_j$$

then Sign_ω changes a sign if and only if for at least $1/2$ of all j $|(0.l_j)_p - (0.\tilde{\omega}^L)_p| \leq 1/L$.⁵ Applying reasoning from the end of section 2.1 we conclude that the actions of I_{E_ω} and \tilde{I}_{E_ω} restricted on $S(a, \omega)$ will differ on less than $\frac{1}{2^{O(v)}}$ and thus this different can be done very small by only linear growth of memory. We thus will omit \sim in our notations.

We define

$$\text{St} = \text{GenArg}^{-1} \text{GenTimeArg}^{-1} (I_{\bar{a}} I_{E_\omega})^t \text{GenTimeArg} \text{GenArg}$$

where GenArg and GenTimeArg generate a pair \bar{a} , $[C]$ and a time instant t correspondingly where C is a gate array implementing $I_{\bar{a}}$. Here the actions of $I_{\bar{a}}$ are implemented by the

⁵We could choose any fixed $\rho : \frac{1}{8} < \rho < \frac{7}{8}$ instead of $1/2$. Really, so defined \tilde{I}_{E_ω} will change the sign of all $\bar{a} \in E_\omega$. If $\bar{a} \perp E_\omega$ then the probability to obtain ω observing the frequency from Rev is less than $\frac{1}{8}$.

universal function of application App. Then the result $\xi = \text{St}|\bar{0}\rangle$ of its action on $\bar{0}$ will be closed to $E_\omega(\bar{a})$. Really, $|\langle E_\omega(\bar{a})|\xi\rangle| = |\sin(2t \arcsin(\langle \bar{a}|E_\omega(\bar{a})\rangle))|$ (look at [BBHT]). An average value of $|\langle \bar{a}|E_\omega(\bar{a})\rangle|$ with the uniformly distributed probability of choice \bar{a} and t over all space and time frame $[0, B]$ correspondingly will be of order $1/\sqrt{N}$. Thus if t is chosen randomly from the uniform distribution over $1, 2, \dots, B$ then $|\langle E_\omega(\bar{a})|\xi\rangle|^2$ will have average value not less than $1/4$. Of course it would be much more convenient to obtain $E_\omega(\bar{a})$ with the error probability converging to zero that is possible by the method described in section 2.1. Namely, arrange h equal registers for the states χ_k , $k = 1, 2, \dots, h$ in the main space, the corresponding h registers for frequencies and associate the variable t_k with each k -th register. Let St_k be a pattern of St operator acting on k -th register. Remind that operators GenArg_k and GenTimeArg_k generate independent distributions for different $k = 1, 2, \dots, h$. Now we define

$$\text{State}^\omega = \text{St}_1 \otimes \text{St}_2 \otimes \dots \otimes \text{St}_h. \quad (2)$$

So defined operator being applied to zero initial state gives a state $\chi_1 \otimes \chi_2 \otimes \dots \otimes \chi_h$ where an average value of $|\langle E_\omega(\chi_k)|\chi_k\rangle|^2$ will be closed to some number not less than $1/4$ with the vanishing probability of error. By the way it means that if we then apply to this state the corresponding operators revealing frequencies: $\text{Rev}_1 \otimes \text{Rev}_2 \otimes \dots \otimes \text{Rev}_h$ then in the resulting state χ the majority of amplitude will be concentrated on such basic states for which at least $\frac{5}{32}$ of all registers for frequencies contain numbers l for which $|(0.l)_m - (0.\tilde{\omega}^L)_p| < 1/L$.⁶ On the other hand, if ω is not a frequency at all then the probability to obtain such basic state will be vanishing in view of independence of distributions generated by GenTimeArg_k and GenArg_k for the different k .

The time complexity of this algorithm is of order $M\sqrt{N} \cdot n^2$. The last multiplier arises due to the copying of registers. Thus we have a solution of the first problem of recognition of eigenvalues.

3.2 Finding thermodynamic functions

Let we are given a structure of molecule of a gas. The problem is to find its thermodynamic function (1). In view of that a summand in this sum quickly converges to zero it is sufficient to find few first summands. Thus it is sufficient to be able to find degree of degeneracy of the subspace corresponding to frequencies $\omega' \approx \omega$ for any $\omega = l/M$. Let $E_0 < E_1 < \dots < E_s$ be energy levels of a molecule or eigenvalues of its Hamiltonian H . Then the operator of evolution in time frame t will be $U = e^{-\frac{iH}{\hbar}t}$. An addition of a diagonal matrix $r \cdot I$ with constant r to a Hamiltonian does not change the physical picture. Then choosing $r = -E_s$, $t = \frac{\hbar}{2\pi E_s}$ we obtain a unitary operator U which frequencies belong to the segment $[0, 1)$ and thus we reduce the problem to the case we have already dealt with.

Assume that M is fixed and we must examine only few frequencies closed to 0. At first we can recognize all numbers of the form l/M that are frequencies in within $1/L$. Let ω be such number. Show how we can find the degree of degeneracy d of the corresponding subspace. This is the dimension of subspace E_ω spanned by eigenvectors corresponding to frequencies $\omega' \approx \omega$.

⁶Note that in this criterion $\frac{5}{32}$ could be replaced by any $\rho : 0 < \rho < \frac{1}{4} \cdot \frac{7}{8} = \frac{7}{32}$.

Our plan is the following. Build an operator I_{E_ω} of reflection along this subspace. Then using a counting procedure built in the paper [BBHT] we evaluate the time required for turning of arbitrary initial vector till this subspace. This time will be about $\sqrt{\frac{N}{d}}$ and thus we find d . Fix some $\epsilon > 0$ and show how to obtain the value of d in within ϵd .

Let operators GenTimeArg_j^a generate time instants t_j from independent uniform distributions on the segment $[0, [a]]$, where a is nonnegative number. For a from 1 to \sqrt{N} fulfil the following loop of three steps:

1. Apply an operator

$$\bigotimes_j \left[\bigotimes_k \text{Rev}_{j,k} \right] (I_{\bar{a}} I_{E_\omega})^{t_j} \text{GenTimeArg}_j^a \text{GenArg}_j$$

2. Find the fidelity of result that is the number of all j for which at least $\frac{7}{8} - \epsilon$ of all k are such that $\omega_{j,k} \approx \omega$. If the fidelity of this step is larger than on the previous, then proceed the loop, if not then stop.
3. Replace a by $4a/3$.

If by the point 2 we finish computation then the current value a is taken as the rough approximation of d from above. We have $3a/4 \leq d \leq a$. To find d more exactly divide the segment $[3a/4, a]$ to $[1/\epsilon]$ equal parts by points $a_0 < a_1 < \dots < a_l$ and repeat the procedure from above sequentially for all a_i . Thus we shall determine d in within $g(\epsilon)d$ where function g quickly converges to zero with ϵ . Thus our algorithm finds d and thermodynamic functions with arbitrary relative error in the time $O(\sqrt{N})M$ where the constant depends on admissible error. The more refined algorithm can be obtained if we apply the method of counting from the work [BHT]. In that work quantum Fourier transform is used analogously to Abrams and Lloyd operator Rev only in order to find a time period of function $G|\xi, t\rangle = |G^t \xi, t\rangle$ that is about $\sqrt{N/d}$. Their method gives the accuracy of order \sqrt{d} which means that the relative error converges to zero if $d \longrightarrow \infty$.

3.3 Recognition of molecular structures

Now take up a problem of recognition of molecular structures. Here we are given a spectrum of molecule and a problem is to recognize its construction. Note that now we have not access to a device but it is sufficient to find an arbitrary device generating this spectrum. Clarify the formulation assuming the following form of determining spectrum. Let we are given a set $\bar{w} = \{w_1, \dots, w_Q\}$ of numbers from $[0, 1)$ of the form $w_i = \frac{l_i}{M}$ each where $l_i \in \{0, 1, \dots, M-1\}$. Denote by F a subspace spanned by vectors of the form $|l_i\rangle$, $i = 1, \dots, Q$. A spectrum S is determined by this set \bar{w} if

- a) for each $\omega \in S$ there exists its good approximation $w_i \in \bar{w}$: $|w_i - \omega| \leq \frac{1}{L}$ and
- b) each $w_i \in \bar{w}$ is a good approximation of some $\omega \in S$.

We would obtain a little different formulations of the problem if we want to find a circuit whose spectrum only contains one given set of frequencies and/or does not contain some other set, or permit some more general form of sparse set for \bar{w} instead of $\frac{l_i}{M}$. These versions of the problem at hand have similar solutions.

As above we shall find a recognizing algorithm in GSA form

$$(I_{\tilde{0}} I_{cir, \bar{w}})^t \quad (3)$$

where $\tilde{0}$ is arbitrarily chosen vector from the space spanned by codes of circuits, $t = O(\sqrt{T})$ where T is a number of all possible circuits, and $I_{cir, \bar{w}}$ is reflection along all such codes $[C]$ that $\text{Spectr}(U_C)$ is determined by \bar{w} . Now it is sufficient to build $I_{cir, \bar{w}}$.

Choose $B_f = O(\sqrt{Q})$ so that a randomly chosen vector $w \in F$ satisfies $|\langle w | w_1 \rangle| > 1/B_f$ with probability 0.99. Let GenFreq_j , GenTimeFreq_j be operators generating correspondingly: a linear combination of frequencies $\tilde{\omega}_j \in F$ and time instant $t_{freq, j} \leq B_f$ - all these objects from the corresponding uniform distributions over all possible values, and a code of gate array generating inversion along the corresponding state $\tilde{\omega}_j$. These operators will generate the objects in the corresponding ancillary registers. Denote by ω_j a frequency contained in the j -th register (that is initially $\tilde{\omega}_j$).

Assume that a code of circuit generating U is fixed. Define an operator $I_{cir, \bar{w}}$ by

$$I_{cir, \bar{w}} = \bigotimes_j \left[\text{GenFreq}_j^{-1} \text{GenTimeFreq}_j^{-1} (I_{BadFreq, \bar{w}, j} I_{\tilde{\omega}_j})^{t_{freq, j}} \text{SignGoodFreq} \right. \\ \left. \bigotimes_j \left[(I_{\tilde{\omega}_j} I_{BadFreq, \bar{w}, j})^{t_{freq, j}} \text{GenFreq}_j \text{GenTimeFreq}_j \right] \right].$$

where $I_{BadFreq, \bar{w}, j}$ will invert a sign of states with "bad frequencies" in j -th register that are such values of ω_j of the form $\frac{l}{M}$, $l \in \{0, 1, \dots, M-1\}$ which either belong to \bar{w} and are not a good approximation of frequencies $\omega \in \text{Spectr}(V)$ or do not belong to \bar{w} but have a closed $\omega \in \text{Spectr}(V)$: $|\omega_j - \omega| \leq \frac{1}{L}$; for all other frequencies this operator acts like identity. Application of the sequence preceding SignGoodFreq concentrates amplitude on "bad frequencies". Note that $I_{\tilde{\omega}_j}$ can be implemented by a given code by means of quantum Klini operator App. The following application of SignGoodFreq inverts a sign of state subject to are there bad frequencies or not. Namely, for codes $[C]$ without bad frequencies SignGoodFreq changes the sign, for codes $[C]$ with bad frequencies it makes nothing. The following operators clean all ancilla. Thus so defined $I_{cir, \bar{w}}$ will invert a sign of exactly those codes C for which $\text{Spectr}(U_C)$ is determined by \bar{w} . We need to define two types of operators: SignGoodFreq and $I_{BadFreq, \bar{w}, j}$.

Associate with each ω_j contained in j -th register the family of registers enumerated by two indices j, k and containing frequencies $\omega_{j,k}$.

Definition 3. Call a family of all $\omega_{j,k}$ good if for at least $1/5$ from all j the following property takes place: for at least $1/10$ of all k $\omega_{j,k} \approx \omega_j \in \bar{w}$.

Registers enumerated by different k for a fixed j are designed for the application of j -th copy of operator State^ω defined in the previous section. Here it has the form State^{ω_j} . Each k corresponds to the operator St_k from the definition (2) so that each $\omega_{j,k}$ will be a frequency obtained from the result of St_k action.

At first build an operator $I_{BadFreq, \bar{w}, j}$. Put

$$I_{BadFreq, \bar{w}, j} = \bigotimes_{j,k} \left[(\text{State}^{\omega_j})^{-1} \text{Rest}_{j,k} \right] \text{Sign}' \bigotimes_{j,k} [\text{Rev}_{j,k} \text{State}^{\omega_j}]$$

where an operator Sign' will change a sign of only states with bad families of frequencies.

If a frequency ω_j is bad then in the previous section it was shown that only for vanishing part of all k we can have $\omega_{j,k} \approx \omega_j \in \bar{w}$ and before Sign' almost all probability will be concentrated on bad families $\omega_{j,k}$, hence $I_{BadFreq, \bar{w}, j}$ changes the sign.

If ω_j is good then it belongs to \bar{w} and has a closed $\omega' \in S$. By the previous section for about $\frac{7}{8} \cdot \frac{1}{4} = \frac{7}{32} > \frac{1}{5}$ of all k will be $\omega_{j,k} \approx \omega \in \bar{w}$ and before Sign' almost all probability will be concentrated on good families, hence the sign will not be changed.

Thus $I_{BadFreq, \bar{w}, j}$ is defined correctly.

Put

$$\text{SignGoodFreq} = \bigotimes_{j,k} \left[(\text{State}^{\omega_j})^{-1} \text{Rest}_{j,k} \right] \text{Sign} \bigotimes_{j,k} [\text{Rev}_{j,k} \text{State}^{\omega_j}]$$

where an operator Sign changes a sign only for states with good families of frequencies. If a frequency ω_j is not bad then for about $\frac{1}{4} \cdot \frac{7}{8} = \frac{7}{32}$ of all k will be $\omega_{j,k} \approx \omega_j \in \bar{w}$. If a frequency ω_j is bad then we can obtain $\omega_{j,k} \approx \omega_j \in \bar{w}$ only for the vanishing part of k as it was shown in the previous section. Thus SignGoodFreq acts how it is needed⁷.

Now calculate the complexity of our algorithm recognizing molecular circuit. The first multiplier \sqrt{T} issues immediately from (3). The following multiplier as \sqrt{Q} issues from the immediate definition of $I_{cir, \bar{w}}$. At last the definition of $I_{BadFreq, \bar{w}}$ brings the multiplier $M\sqrt{N}$. The resulting complexity will be of order $M\sqrt{TNQ}n^2$.

3.4 Distinguishing of eigenvectors of two operators with the same eigenvalue

Now we are going to take up the most difficult of our problems - a problem of recognition of electronic devices. The difficulty is that here we need not to find a circuit with given spectrum but to simulate an action of given circuit. Remind that now we assume that frequencies can be determined in within $1/L$ given their approximation in within $1/M$ where $L \gg M$.

As a first step we consider the following question. Given two operators U and V having the same eigenvalue ω how to find a difference between the corresponding eigenvectors? Let L_ω^U, L_ω^V be the subspaces spanned by eigenvectors of U and V corresponding to all frequencies $\omega' \approx \omega$. (A particular case is when ω is a frequency of U but not of V . Here $L_\omega^V = \emptyset$ and our algorithm will work in this situation.) We shall omit the index ω in the notations. For $u \in L^U, \|u\| = 1$ put

$$\mu_u = \min\{\sqrt{1 - |\langle u|v \rangle|^2} \mid v \in L^V, \|v\| = 1\}.$$

⁷Again we could take arbitrary $\rho_1 : 0 < \rho_1 < 1$ instead of $\frac{1}{10}$ and $\rho_2 : 0 < \rho_2 < \frac{7}{32}$ instead of $1/5$ in the definition of a good family.

that is the sine of angle between a vector u and the subspace L^V or a distance between u and this subspace, and analogously define μ_v for $v \in L^V$, $\|v\| = 1$.

Put

$$\mu_U = \max_{u \in U} \mu_u, \quad \mu_V = \max_{v \in V} \mu_v.$$

Then say $\mu_U = 0$ means that $U \subseteq V$. If the dimension of spaces L^U, L^V are equal then $\mu_U = \mu_V$, if they are not equal, say $\dim L^U > \dim L^V$ then $\mu_U = 1$.

Let $d = d(N)$ be some function taking values from $(0, 1]$.

Call these subspaces d - distinguishable if some of μ_U, μ_V is not less than d , or some of the subspaces is empty and another is nonempty.

We shall build a procedure that determines are these subspaces the same or not provided they can be either d - distinguishable or coincident. The less the function $d(N)$ is the more accurate our recognition will be. Let $L^U \cap L^V = L_0$. Then $L^U = L_0 \oplus L'_U$ and $L^V = L_0 \oplus L'_V$. Note that if $L'_U \neq \emptyset$ then for all vectors from L'_U of the length 1 their distances from L^V are exactly μ_U and the same thing takes place with L^V if L'_V is not empty. Let L' be linear subspace spanned by vectors from $L'_V \cup L'_U$. Denote by $\text{Proj}_A B$ a projection of subspace B to subspace A . If $\dim L^U > \dim L^V$ then we have the following expansion to the sum of orthogonal subspaces: $L^U = L''_U \oplus \text{Proj}_{L^V} L^U$, where L''_U is a subspace in L^U consisting of vectors orthogonal to L^V . Let L''_V be defined symmetrically.

Then either

- $L^U = L^V$ or
- $\dim L^U = \dim L^V$ and $L' \neq \emptyset$, or
- $\dim L^U > \dim L^V$ and $L''_U \neq \emptyset$, or
- $\dim L^U < \dim L^V$ and $L''_V \neq \emptyset$.

We define the main operator determining the equality of L^U and L^V by

$$\begin{aligned} \text{Difference} &= \text{Differ}^{-1} \text{SignDif Differ}, \\ \text{Differ} &= \text{Dif}_{\text{same dim}} \text{Dif}_{L^U > L^V} \text{Dif}_{L^U < L^V} \text{Dif}_{L^U > L^V}^{\text{ort}} \text{Dif}_{L^U < L^V}^{\text{ort}} \end{aligned} \quad (4)$$

where SignDif changes a sign of main ancilla α_{dif} iff at least one ancilla from the list $\bar{\alpha} = \{\alpha_{\text{same dim}}, \alpha_{L^U > L^V}, \alpha_{L^U < L^V}, \alpha_{L^U > L^V}^{\text{ort}}, \alpha_{L^U < L^V}^{\text{ort}}\}$ contains 1, and each operator of the sort Dif changes the corresponding ancilla from $\bar{\alpha}$ in cases

- $\dim L^U = \dim L^V$ and $L^U \neq L^V$,
- $\dim L^U > \dim L^V$ and $\mu_V < \sqrt{2/3}$,
- $\dim L^U < \dim L^V$ and $\mu_U < \sqrt{2/3}$,
- $\dim L^U > \dim L^V$ and $\mu_V > \sqrt{1/3}$, or $L^V = \emptyset$,

- $\dim L^U < \dim L^V$ and $\mu_U > \sqrt{1/3}$, or $L^U = \emptyset$

correspondingly and all of them do nothing if $L^U = L^V$. In view of symmetry it is sufficient to define Dif operators in the first, second and fourth cases. Note that the first case $\dim L^U = \dim L^V$ is the only non-degenerate case and the definition of Dif here will be the most difficult.

Definition of $\text{Dif}_{\text{same dim.}}$

Suppose that $\dim L^U = \dim L^V$. Our first aim now is to build an operator Inv which acts as identity if L^U and L^V are coincident and acts like $I_{L'}$ if they are d - distinguishable. Arrange the first two ancillary qubits α_U, α_V which will signal that a state at hand has a projection at least of the length $1/3$ to L^U or, correspondingly to L^V . Consider the following operator

$$\text{Check} = \bigotimes_s \text{Rest}_s^V \text{Anc}_V \bigotimes_s \text{Rev}_s^V \bigotimes_s \text{Rest}_s^U \text{Anc}_U \bigotimes_s \text{Rev}_s^U$$

where Anc inverts the corresponding ancilla if and only if at least nine tenth of copies for the respective frequencies are equal to ω in within $1/M$. It coincides with the inverse operator Check^{-1} .

Let t be some random integer from the segment $[0, \lfloor \frac{2}{d} \rfloor]$. We define the following operator of Grover's type:

$$\text{Turn}_t = (I_{L^U} I_{L^V})^t \quad (5)$$

Call two subspaces L^U and L^V almost orthogonal iff for some $\mu \in \{\mu_U, \mu_V\}$ $\sqrt{1 - \mu^2} \leq 1/30$. If L^U and L^V are not almost orthogonal then given some $a \in L'_U$ ($a \in L'_V$) an average distance between $\text{Turn}_t|a\rangle$ and L_U (L_V) will be at least $1/2$ if L^U and L^V are d - distinguishable and zero if these subspaces are coincident. To tell apart close location and almost orthogonality build two operators: Dist_{ort} and $\text{Dist}_{\text{closed}}$.

At first suppose that L^U and L^V are almost orthogonal. Then $\alpha_U = 1$ means that $\alpha_V = 0$. Introduce a notation

$$L(\alpha_U, \alpha_V) = \begin{cases} L^V, & \text{if } \alpha_U = 1, \\ L^U, & \text{if } \alpha_V = 1. \end{cases}$$

Let \bar{a} be a vector at hand from the space of inputs. Note that if $L^U \neq L^V$ then for each $\bar{a} \perp L'$ we shall have $\alpha_U = \alpha_V$ because such \bar{a} belongs to the subspace spanned by L_0 and orthogonal subspace to $L^U \cup L^V$. The first operator Dist_{ort} will do nothing if $\alpha_U = \alpha_V$ and will change a sign and a special ancilla α_{ort} if a projection of \bar{a} to $L(\alpha_U, \alpha_V)$ is less than $1/30$.

The second operator $\text{Dist}_{\text{closed}}$ will act like identity if $\alpha_U = \alpha_V$ and will change a sign in case when the following conditions are satisfied simultaneously: $\bar{a} \in L'$, L^U and L^V are distinguishable, $\alpha_{\text{ort}} = 0$.

Put

$$\text{Dist}_{\text{ort}} = \bigotimes_j \text{Res}_j \text{Si}_{\neq \omega} \bigotimes_j \text{Re}_j$$

where Re (Res) denotes Rev^V (Rest^V) if $\alpha_U = 1, \alpha_V = 0$, Rev^U (Rest^U) if $\alpha_V = 1, \alpha_U = 0$, and identity if $\alpha_U = \alpha_V$; $\text{Si}_{\neq \omega}$ changes a sign inverting simultaneously α_{ort} iff at least a half of frequencies ω_j are such that $|\omega_j - \omega| > 1/M$ and $\alpha_U \neq \alpha_V$. If we want to clean the second

ancilla after the action of Dist_{ort} and remain change in sign then we can use an operator $\text{Dist}_{ort}^- = \bigotimes_j \text{Res}_j S_{\neq \omega} \bigotimes_j \text{Re}_j$ where S acts like Si only without changing a sign.

The second operator will be defined by the following equations

$$\begin{aligned} \text{Dist}_{closed} &= D_1^{-1} \dots D_n^{-1} S' D_n D_{n-1} \dots D_1, \\ D_j &= (\text{GenTimeArg}_j)^{-1} (\text{Turn}_{t_j}^j)^{-1} \left[\bigotimes_k \text{Rest}_{j,k}^U \right] \text{Sig}_{\neq \omega}^j \left[\bigotimes_k \text{Rev}_{j,k}^U \right] \text{Turn}_{t_j}^j \text{GenTimeArg}_j \\ j &= 1, 2, \dots, n, \end{aligned}$$

where operator $\text{Sig}_{\neq \omega}^j$ changes the corresponding ancilla β_j only in one of the two cases:

- 1) $\alpha_U = 1$ and at least a half of $\omega_{j,k}$ are such that $|\omega_{j,k} - \omega| \geq 1/M$, or
- 2) $\alpha_U = 0$, $\alpha_V = 1$ and at least a half of $\omega_{j,k}$ are such that $|\omega_{j,k} - \omega| < 1/M$.

An operator S' changes a sign iff some of α_U, α_V is nonzero and at least $1/20$ of all β_j contain 1.

Consider the action of Dist_{closed} following to Check on an input vector \bar{a} . Let at first $L^U \neq L^V$ which means that they are distinguishable.

If $\bar{a} \perp L^U, L^V$ then $\alpha_U = \alpha_V = 0$ and Dist_{closed} makes nothing.

If $\bar{a} \in L_0$ then $\alpha_U = \alpha_V = 1$ and all $\text{Sig}_{\neq \omega}^j$ makes nothing because for almost all j about $3/4$ of $\omega_{j,k}$ are closed to ω : $|\omega_{j,k} - \omega| \leq 1/M$, hence S' and Dist_{closed} do nothing.

Let $\bar{a} \in L'$. Prove that Dist_{closed} changes a sign. Expand L' to the sum of orthogonal subspaces: $L' = L'_U \oplus L'^{ort}_U$. Denote the result of action of $\text{Turn}_{t_j}^j$ on \bar{a} by \bar{a}_j .

If $\bar{a} \in L'_U$ then $\alpha_U = 1$, and for more than $1/10$ of all \bar{a}_j revealed frequencies are not closed to ω with probability about $\frac{3}{4} \cdot \frac{9}{10}$, hence a sign will be changed by the point 1).

If $\bar{a} \in L'^{ort}_U$ then by the same reason we obtain the change of sign by the point 2). Hence Dist_{closed} changes a sign for all $\bar{a} \in L'$.

Now we can define Inv:

$$\text{Inv} = \text{Check} \text{Dist}_{ort}^- \text{Dist}_{closed} \text{Dist}_{ort} \text{Check}.$$

For $\bar{a} \perp L^U, L^V$ we have $\text{Inv}|\bar{a}\rangle = |\bar{a}\rangle$ because Check gives zero in ancilla α_U, α_V thus depriving the following operators ability to change somehow a state vector. If $\bar{a} \in L_0$ then $\text{Inv}|\bar{a}\rangle = |\bar{a}\rangle$ because Dist_{ort} makes nothing and Dist_{closed} makes nothing as well. Thus $\text{Inv}|\bar{a}\rangle = |\bar{a}\rangle$ for $\bar{a} \perp L'$, and $\text{Inv}|\bar{a}\rangle = -|\bar{a}\rangle$ for $\bar{a} \in L'$.

Now we are ready to build an operator $\text{Dif}_{same \ dim}$ inverting the ancilla $\alpha_{same \ dim}$ if and only if L^U and L^V are distinguishable. Let Gen generate a list $y, [I_y], [C_Z]$ where $[C_Z]$ is a code of circuit generating some unitary operator $Z = Z^{-1}$ having only eigenvalues 1 and -1 that is its frequencies are 0 and $1/2$ and the space corresponding to frequency 0 is one dimensional where y is its basic vector. As usually index j means that the corresponding vectors y_j are taken from the uniform distribution on all possible vectors. Assume that operators of the form Gen^{-1} are accessible for us as well. Put

$$\begin{aligned} \text{Dif}_{same \ dim} &= \bigotimes_j \left[\text{GenTimeArg}_j^{-1} \text{Gen}_j^{-1} (\text{Inv}_j I_{y_j})^{t_j} \text{Rest}_j^{Z_j} \right] \text{Change} \\ &\quad \bigotimes_j \left[\text{Rev}_j^{Z_j} (I_{y_j} \text{Inv}_j)^{t_j} \text{Gen}_j \text{GenTimeArg}_j \right] \end{aligned} \tag{6}$$

where each copy of Inv acts on the register where initially is placed y_j , Change makes a desired change in a resulting qubit $\alpha_{\text{same dim}}$ provided at least $5/32$ of all frequencies differ from 0 in more than $1/M$.

The group $(I_{y_j} \text{Inv}_j)^{t_j}$ of GSA type turns essentially a vector y_j generated by Gen_j if and only if L^U and L^V are d -distinguishable.

If $L^U = L^V$ then y_j remains unchanged and at least $7/8$ of all frequencies will be closed to 0.

If $L^U \neq L^V$ then for the result of the turn of y_j at least $\frac{7}{8} \cdot \frac{1}{4} = \frac{7}{32}$ of frequencies will be far from 0 because they must be closed to $1/2$.⁸

Definition of $\text{Dif}_{L^U > L^V}$.

Suppose that $\dim L^U > \dim L^V$ and $\mu_V < \sqrt{2/3}$. Remind that here we have an expansion to the sum of orthogonal subspaces $L^U = L''_U \oplus \text{Proj}_{L^U L^V}$ where $L''_U \neq \emptyset$. We shall define the operator Dif by a very similar way as in previous case:

$$\begin{aligned} \text{Dif}_{L^U > L^V} = & \bigotimes_j \left[\text{GenTimeArg}_j^{-1} \text{Gen}_j^{-1} (\text{Inv}_{j,U}'' I_{y_j})^{t_j} \text{Rest}_j^{Z_j} \right] \text{Change} \\ & \bigotimes_j \left[\text{Rev}_j^{Z_j} (I_{y_j} \text{Inv}_{j,U}'')^{t_j} \text{Gen}_j \text{GenTimeArg}_j \right] \end{aligned}$$

where the definition of Inv_U'' inverting L''_U looks like Dist_{ort} only L''_U will play a role of L' :

$$\text{Inv}_U'' = \text{Check} \left[\bigotimes_k \tilde{\text{Res}}_k^V \right] \tilde{\text{Si}}_{\neq \omega} \left[\bigotimes_k \tilde{\text{Re}}_k^V \right] \text{Check}.$$

Here $\tilde{\text{Re}}^V$ and $\tilde{\text{Res}}^V$ act like Rev^V and Rest^V only if $\alpha_U = 1$ and if $\alpha_U = 0$ then they do nothing, $\tilde{\text{Si}}_{\neq \omega}$ changes a sign only in one case: if $\alpha_U = 1$ and at least $3/4$ of all frequencies ω_k are far from ω : $|\omega_k - \omega| \geq 1/M$. Thus in Dif operator we shall use a set of ancillary registers enumerated by pairs of indices j, k .

For $\bar{a}_j \in \text{Proj}_{L^U L^V}$ in view of $\mu_V < \sqrt{2/3}$ an operator $\tilde{\text{Si}}_{\neq \omega}$ does not change a sign because here the fraction of all frequencies closed to ω is $\frac{7}{8} \cdot \frac{1}{3} = \frac{7}{24} > \frac{1}{4}$.

For $\bar{a}_j \perp \text{Proj}_{L^U L^V}$ an operator Inv_U'' makes nothing.

Definition of $\text{Dif}_{L^U > L^V}^{\text{ort}}$

Suppose that $\dim L^U > \dim L^V$ and $\mu_V > \sqrt{1/3}$. The definition of Dif will be similar to the previous case only the whole subspace L_U will play a role of L' :

$$\begin{aligned} \text{Dif}_{L^U > L^V}^{\text{ort}} = & \bigotimes_j \left[\text{GenTimeArg}_j^{-1} \text{Gen}_j^{-1} (\text{Inv}_{j,U} I_{y_j})^{t_j} \text{Rest}_j^{Z_j} \right] \text{Change} \\ & \bigotimes_j \left[\text{Rev}_j^{Z_j} (I_{y_j} \text{Inv}_{j,U})^{t_j} \text{Gen}_j \text{GenTimeArg}_j \right] \end{aligned}$$

where

$$\text{Inv}_U = \text{Check} \left[\bigotimes_k \tilde{\text{Res}}_k^V \right] \tilde{\text{Si}}_{\neq \omega}^{\text{ort}} \left[\bigotimes_k \tilde{\text{Re}}_k^V \right] \text{Check}.$$

⁸Thus we could take any number ρ : $\frac{1}{8} < \rho < \frac{7}{32}$ instead of $\frac{5}{32}$ in the definition of Change .

Here $\tilde{S}_{\neq\omega}^{ort}$ changes a sign if more than a half of frequencies are far from ω : $|\omega_j - \omega| > 1/M$. The satisfying of the conditions required for Dif operator is based now on inequality $\frac{7}{8} \frac{2}{3} = \frac{7}{12} > \frac{1}{2}$ and can be checked straightforwardly.

At last estimate the complexity of constructed procedure. An operator Turn (5) requires of order $\text{Turn}_{complexity} = M\sqrt{1/d}$ elementary steps. Then, Difference (4) requires of order $\text{Turn}_{complexity}\sqrt{N}$ that is $O(M\sqrt{N/d})$ elementary steps. Note that there exists the similar form of operator Difference which does not act on resulting qubit α_{dif} but changes a sign instead and such operator can be constructed similarly. Denote this operator by Difference_{sign} . Assume that an input of it contains a frequency ω .

3.5 Recognition of electronic devices circuits

Now we are ready to take up the recognition of circuits. We assume that for every pair of circuits for their transformations U_1, U_2 subspaces spanned by corresponding eigenvalues are either coincident or d -distinguishable. Assume also that our coding procedure gives one-to-one correspondence between circuits and T basic states e_0, e_1, \dots, e_{T-1} in the space H_{cir} . Recognizing procedure is denoted by Rec and will have the GSA form:

$$\text{Rec} = (I_{\tilde{0}} I_U)^t, \quad t = O(\sqrt{T}) \quad (7)$$

acting on states of the form $|\chi\rangle$ where basic states for χ are codes of circuits. Here $\tilde{0} \in H_{cir}$ is chosen arbitrarily and I_U inverts a sign of every code which circuit induces a given operator U . An implementation of $I_{\tilde{0}}$ is straightforward and all that we need is to build I_U .

We define I_U as

$$I_U = \bigotimes_j [\text{Conc}_{freq, j}^{-1} \text{Difference}_j] \text{Sign} \bigotimes_j [\text{Difference}_j \text{Conc}_{freq, j}]$$

where Conc_{freq} for every basic state C of argument will generate some arbitrary distribution of amplitude on ancillary register with Q basic states and then will concentrate substantial part of amplitude on a frequency ω for which L^U and L^V are distinguishable (if such frequency exists). Then operator Difference_j changes resulting qubit for j th copy if and only if on this frequency these subspaces are distinguishable. The following operator Sign changes a sign if and only if at least one fifth of resulting qubits α_{dif} contain 1, e.g. if and only if operators U and U_C are the same. Then the following applications of Difference_j to each copy of register clean the corresponding resulting qubits and inverses operators for Conc_j restore an initial state of ancillary register. Difference was constructed in the previous section and all we need now is to build $\text{Conc}_{freq, j}$. This transformation can be defined as

$$\text{Conc}_{freq, j} = \text{GenTimeFreq}_j^{-1} \text{GenFreq}_j^{-1} (\text{Difference}_{sign} I_{\omega_j})^{t_j} \text{GenFreq}_j \text{GenTimeFreq}_j \quad (8)$$

If U and U_C are different then by our assumption for some ω their subspaces L^U and L^V are d -distinguishable then Conc_j will concentrate substantially large part of amplitude over all j on some combination of such values ω . Thus we have constructed a required procedure Rec

which gives a target code with substantial probability as a result of observation of the register for code C . After the observation we can verify a fitness of a code found C by a straightforward procedure. It is similar to I_U with the single change: Sign will be replaced by change in a special ancilla which can be observed after procedure and thus we shall learn does a code C at hand fit or not.

What is the complexity of our procedure Rec? The complexity $Mn^2\sqrt{N/d}$ of Difference must be multiplied by \sqrt{Q} issued from (8) and by \sqrt{T} issued from the immediate definition (7). The resulting complexity will be $Mn^2\sqrt{TQN/d}$.

3.6 Advantages of the recognizing algorithms

Advantages of the proposed algorithms are connected with their high speed and small memory. Particularly, the algorithm for molecular structures recognition makes possible to recognize molecular circuits using microscopic memory whereas classically this task requires exponentially large memory. Compare the proposed algorithms with their classical counterparts. We shall omit logarithmic multipliers.

1. Recognition of eigenvalues and finding thermodynamic functions. Fix some value of M determining a precision of eigenvalue approximation. Consider at first the case when the number of ancillary qubits in a quantum gate array at hand is small. Then by the direct classical method we must build a matrix of unitary transform induced by a gate array. It requires of order N^3 steps and at least of order N^2 bits. The known quantum algorithm given by Travaglione and Milburn in [TM] basing plainly on Abrams and Lloyd operator Rev contains repeated measurements of frequencies hence it requires the time of order NM - for sparse spectrums it is of the same order as for Hams-Raedt algorithm and its only advantage over the last is exponential memory saving.

Our algorithm recognizes an eigenvalue in $\sqrt{NM}n$ steps. This time for the sparse area of spectrum is about square root of the time of best known algorithms. Here the memory will be of order g^2 qubits (g is the size of gate array), that is about squared memory used in [AL] but still exponentially smaller than of classical methods. Thus the proposed algorithm gives essential speedup over known methods in case when the number of ancillary qubits in a given gate array is small (as in case of molecular structure simulated by gate array) and an area of spectrum at hand is sparse. The same advantage we have with the proposed method of finding thermodynamic functions.

If spectrums are dense we assume that $M = N$ which means that eigenvalues differ at least on $1/N$. Then the time of our algorithm is $O(N)$.

Consider the case when the number a of ancillary qubits involved simultaneously in the gate array is much more than the length n of input. Then the direct classical method requires more than 2^{2a} steps and at least 2^m bits whereas our algorithm requires only about $g2^n$ steps and gn^2 memory and the quantum speedup may be more than square root.

2. The recognition of molecular structures. At first assume that spectrums are sparse. To be able to compare our method with the evident classical algorithm let us assume that a code of molecular circuit of the length n is a string of ones and zeroes of this length. Thus $M = N$. The

next natural assumption that may be also presumed for electronic circuits is that the sampling of a code of circuit from the uniform distribution induces a sampling of all possible spectrums from the uniform distribution as well. Then the number of all possible choices of spectrums approximations (or parts of spectrum subject to the statement of recognition problem) in within $1/L$ consisting of frequencies of the form l/M is about $2^M = N$. It means that in our assumption M and Q must be logarithmic of N . Hence our method has the time complexity $O(N)$. With these assumptions the time complexity of the classical direct algorithm examining all codes and calculating the corresponding spectrums is about $N^3 \cdot N = N^4$ whereas our algorithm requires the time about N and logarithmic memory. Thus the quantum time for this problem is about fourth root of the time of classical direct method and quantum space is logarithmic.

If spectrums are dense then Q and M will be of order N and our method requires the time $O(N^{2.5})$ comparatively with $O(N^4)$ of direct classical way.

3. Recognition of electronic devices. Here in the general case there are no classical analogs. Compare two algorithm constructed above with their classical and known quantum counterparts. At first consider the single recognizing quantum algorithm that can be easily deduced from the technique known before. This is an algorithm of recognizing a circuit realizing classical involutive function of the form $f : Q \longrightarrow Q$, $f = f^{-1}$. This task can be reduced to the search of y such that the following logic formula is true: $\forall x A(x, y)$ where $A(x, y)$ is some predicate. Indeed, if we take $Y(x) = U(x)$ in place of $A(x, y)$ where Y is a function whose code is y then we just obtain the problem of recognition of circuit generating U . An algorithm for such formulas given in [BCW] has the time complexity of order \sqrt{TN} . This task is a particular case of our algorithm for involutive devices and it has the same complexity. In this particular case quantum time is of order square root of classical. But if we regard a bit more general but still restricted problem of recognition of involutive devices producing linear combinations of basic states (like quantum subroutines) an advantage over classical method of recognition will be more. For example, consider the restricted problem when we must choose between two alternative constructions of a tested device inducing not classical unitary transformation. The naive method of observing the results of action of a tested device on the different inputs requires of order $\frac{1}{\epsilon} N^3$ steps to restore the matrix of the operator U_C in within ϵ . Then this ϵ must be less than $1/\sqrt{N}$ to give vanishing difference between operators in Hilbert space. Hence the time complexity of the naive method of recognition is roughly $N^{7/2}$. On the other hand the method proposed in the section 3.4 requires the choice of d only converging to zero with N converging to infinity. Thus the time required by our method is a little more than \sqrt{N} . We thus have almost seventh degree speedup for the problem of distinguishing electronic circuits generating transformations with not classical matrices.

4 Conclusion

The main conclusion is that molecular structure and physical properties of environment can be quickly recognized on the microscopic level whereas the classical methods require huge time and especially memory. The new algorithms recognizing eigenvalues with fixed precision and molecular structure, finding thermodynamic functions give a quadratic speedup comparatively

with the best classical algorithms and exponential memory saving. The new method based on quantum computing was proposed for fast recognition of electronic devices. By this method two devices with the same given spectrum can be distinguished in the time about seventh root of the time of direct measurements. All these algorithms show essential potential advantages of microscopic sized quantum devices comparatively with their classical counterparts with much bigger memory. The advantages touch intellectual tasks like recognition of the structure of other devices and important properties of environment. The proposed algorithms are built of standard known subroutines; they have simple structure and lay completely in the framework of conventional paradigm of quantum computing.

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